Indian J. Phys. 43, 700—702 (1969)

Letters to the Editor

Probability-operator of a quantum system for thermodynamics.*

By M. Dutta

Centre of Advanced Studies in Applied Mathematics, University of Calcutta, Calcutta-9, India.

(*Received* 28 *August* 1969)

Essentially statistical investigations of a physical system with two fundamental entities, which are additive, numerically measurable, but random in nature were made by Dutta (1953, '55, '59, '60, '65, '66) for solving the main problem of (equilibrium) thermodynamics. The probability distribution for the measured values of the fundamental entities were written by arguments similar to those used for Bayes' rule or for writing the likli-hood-function after Fisher and then parameters were estimated by the method of maximum likelihood. From the equation for conservation of any one of the fundamental entities, the known results of statistical thermodynamics were deduced. Afterwards it was shown (Dutta 1966) that additivity of fundamental entities leads to an exponential (a canonical or a grand canonical) law for distributions in statistical physics. The entire discussion may be equally applicable to a system, composed of a large number of constituent microscopic parts or to a single macroscopic system with some entities of which the total measure may fluctuate at random. A purely probabilistic treatment of thermodynamic problems is also due to Jaynes (1957).

A system like quantum liquid (viz. liquid helium) is essentially a quantum (macro-) system (Landau & Lifshitz 1969). Also, a system with strong interactions amongst its constituent parts is usually considered as a single quantum system. So, it is necessary as well as interesting to see how to modify the discussions of essentially statistical theory of thermodynamics, consistently with the usual formalism of quantum mechanics, *i.e.* in terms of Hilbert space and linear operators on it, so that an essentially quantum system may be duly investigated. The present note is an attempt in that direction.

For a quantum system, the states are represented by points of a Hilbert space, $\boldsymbol{H}$, and any physical (dynamical) variable is a Hermitean linear operator on $\boldsymbol{H}$ into $\boldsymbol{H}$ (Dirac 1936, von Neumann 1955). Measured values of a physical variable are eigen-values of the corresponding linear operator.

*A brief synopsis of this note was accepted by the International Conference on Statistical Mechanics held at Kyoto (Japan) in September 1968.

Now, in statistical investigations, to a set of measured values of fundamental physical entities, a probability-distribution is associated. If the probability is also taken as a measurable physical quantity, a linear operator $\boldsymbol{P}$ on $\boldsymbol{H}$ is to be associated with it. To take account of the statistical distribution associated with a thermodynamic system, von Neumann (1955) also introduced a linear operator $\boldsymbol{U}$ on $\boldsymbol{H}$, named by him as the statistical operator.

As the probability is a function of the measured values of fundamental entities like energy etc., so $\boldsymbol{P}$ is a function of operators corresponding to them, viz., Hamiltonian etc. The product rule of probabilities of independent random variables implies multiplicative property of $\boldsymbol{P}$ and operators like Hamiltonian etc., representing fundamental physical quantities for independent systems are commutative in the cartesian product of Hilbert spaces of states of those independent systems and the total Hamiltonian is the sum of two Hamiltonians of constituent parts. Now, $\boldsymbol{P}$ is an operator valued function of the Hamiltonians, $\boldsymbol{H}$'s, and is multiplicative for the statistically independent systems. As statistical independence implies absence of interactions, so for the statistically independent systems, $\boldsymbol{H}$'s are evidently commutative and the total Hamiltonian is the sum.

Now, Hilbert space is also a Banach space and a space of linear operators on a Banach space to a Banach space is also a Banach space. Moreover, as linear operators representing physical (dynamical) variable are endomorphisms of $\boldsymbol{H}$, so they form a Banach algebra. It is well-known that in a Banach algebra $\boldsymbol{B}$, the functional equation

$$\boldsymbol{P}(H_1 + H_2) = \boldsymbol{P}(H_1) + \boldsymbol{P}(H_2),\ H_1, H_2, \boldsymbol{P}(H_1), \boldsymbol{P}(H_2)\ \Sigma\ \boldsymbol{B}$$

is satisfied by

$$\boldsymbol{P}(H) = j \exp(L(H))$$

where j is an idempotent, $L(H)$ is a linear on $\boldsymbol{B}$, to itself and j, $L(H_1)$, $L(H_2)$ commute for all H_1, $H_2\ \Sigma\ \boldsymbol{B}$. Now, the simplest form of $L(H)$ is taken as $\prec H$ where due to the Hermiticity of the operators, $\prec$ is real. If j be taken as the unit element e one gets

$$\boldsymbol{P}(H) = \exp(\prec H)$$

This expression agrees with that for the statistical operator of von Neumann obtained for a system composed of a large number of simple quantum constituents by methods partly quantum mechanical and partly thermodynamic. In this case, the conditions of statistical (thermodynamic) equilibrium will yield as a function of temperature etc., characteristics of thermodynamic equilibrium. If j be taken as the null element θ, $\boldsymbol{P}(H) = \theta$ and this solution appears to be physically untenable. If $\boldsymbol{B}$ contains idempotent

elements other than θ and e and j represent one of them (not θ nor e) one gets,

$$P(H)=j \exp(\alpha H)=j \exp(\alpha jH), \ (\alpha \text{ real})$$

as j also commutes with H. This result appears to be new and interesting and the investigation of its full significance will be the subject matter of a future work. Here, it may only be pointed that as j, $L(H)$ etc. commute with H's, so the argument of exponential must be some constant of motion associated with the system ; in this respect the result appears to be similar to the general probability distribution proposed by Gibbs (1902) for the classical cases.

In order that the above theorem is applicable, H_1 and H_2 should have values in a closed subset of the Banach space formed by the linear operators on H. This will be realisable if the systems (1) and (2), of which one is a system under consideration and the other is the surroundings, be looked upon like heat-bath and matter-bath which can interchange their constituents freely within a suitable range as in the corresponding cases, discussed earlier (Dutta, 1965). The assumption of the existence of a set of values of H_1 and H_2 leads to the hypothesis of the resolution of the Hilbert space, the direct sum of the Hilbert spaces of the systems (1), (2) in a large number of different ways. This point requires a careful mathematical scrutiny which will be investigated later.

References

Dirac, P.A.M. 1947 *The Principles of Quantum Mechanics*, 3rd edition, Oxford University Press.

Dutta M. 1953*a* *Bulletin of Int. Stat. Inst.* **32**, 268.

1953*b* *Proc. Nat. Inst. Sc. (Ind)* **19**, 109.

1955 *Proc, Nat. Inst. Sc. (Ind.)* **21**, 373.

1960 *Gnan O Bignan (in Bengali)* **13**, 737.

1965 *Zeit. f. Phys. Chemie* **228**, 380.

1966 *Indian J. Phys.* **40**, 85.

1969*a* *Proc. Sum. Inst. of Theor. Physics at Mussourie (India)* 231.

1969*b* *Statistical Physics (Foundation)*, World Press (India), (in Press).

Gibbs, J. W. 1902 *Elementary Principles of Statistical Mechanics*, Yale University Press, New Haver, USA.

Hille, E. 1957 *Functional Analysis and Semigroups, Amer. Math. Soc. Publications* (1957).

Jaynes, E. T. 1957 *Phys. Rev.*, **106**, 620, and **107**, 171.

Landau, L. D. & Lifshitz, E. M. 1959 *Statistical Physics*, Pergamon Press., U. K.

Von Neumann, John 1955 *Mathematical Foundation of Quantum Mechanics*, Princeton University Press, U.S.A.